FALL3D-7.1

USER'S MANUAL

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1 Introduction

FALL3D-7.1 is a 3-D time-dependent Eulerian model for the transport and deposition of tephra. The model solves a set of advection-diffusion-sedimentation (ADS) equations on a structured terrain-following grid using a second-order Finite Differences (FD) explicit scheme.
The model inputs are meteorological data, topography, vent coordinate, Eruption Source Parameters (ESP) such as column height, Mass Flow Rate (MFR), eruption duration, and Total Grain-Size Distribution (TGSD) which include particle shape and density information. Outputs are tephra ground load/thickness, airborne ash concentration and other related variables.
The code, written in FORTRAN-90, is available for Unix/Linux/Mac X Operating Systems (OS) and can be compiled either as serial or parallel using MPI. A set of pre- and post-process utility programs and related scripts are also included in the FALL3D-7.1 distribution package.
Several parameterizations can be chosen to describe eruption source geometry and physics, particle terminal settling velocity, eddy diffusivity tensor, and ash aggregation.
For the meteorological variables FALL3D-7.1 uses an off-line strategy, *i.e.* variables are furnished by independent meteorological models or datasets and interpolated to the FALL3D-7.1 grid as NetCDF files.
The FALL3D-7.1 model can be used to reproduce features of past eruptions, as a tool for short-term ash dispersal forecasting, and for volcanic fallout hazard assessment.

2 New features in FALL3D-7.1

Relevant changes have been introduced in FALL3D-7.1. The main new features added to FALL3D-7.1 include:

- A unified source code for both serial and parallel versions (only the serial version was available for public distribution in previous releases);
- The possibility of using forecasts/reanalysis meteorological data from several global/meso-scale meteorological models (not available for public distribution in previous releases);
- Different parameterizations available for ash aggregation. For computational reasons, a preliminary Total Grain Size Distribution (TGSD) file (furnished either by the user or generated by the preprocess SETTGSD utility program) is modified in order to create the final "effective" granulometry file filename.grn which can include an aggregated class and a volatile species, treated as tracers;
- An option describing the cloud spreading at the Neutral Buoyancy Level (NBL) for large eruptions using a semi-analytical gravity current model;
- New parameterizations for resuspension of deposited volcanic ash by wind;
- A parameterization to account for wet deposition;
- Two new parameterizations to estimate cross-wind effects on Mass Flow Rate (MFR);
- A new multi-platform installation method that utilizes the configure command option. The program can be installed on different machines sharing the same filesystem or on a single machine that has different compilers.

With respect to FALL3D-7.0 the new version FALL3D-7.1 differs for:

- A bug in the calculation of particle densities was corrected in the subroutine setfrac.f90 used by the utility program SetTgsd;
- A bug in the utility program SetDbs when used with option profile was corrected;
- A few bugs were corrected in the subroutine costa.f90 used by the utility program SetSrc;
- A few bugs in the Scripts for generating the meteorological database were corrected;

- A new variable (MIXING_FACTOR), specifying the relative weight of grain-size sub-populations, was added in the block GRANULOMETRY block of the input file read by the utility SetTgsd (if this parameter is not specified when BIGAUSSIAN option is specified is set to its default value 0.5);
- The subroutine solveplume.f90, used by the utility program SetSrc, was modified to better describe the plume velocity above the Neutral Buoyancy Level;
- The utility Fall3d2GMT uses a new variable (DEPOSIT_DENSITY_(KG/M3)) in the block POSTPROCESS of the input file for specifying the deposit density (by default DEPOSIT_DENSITY_(KG/M3) =1000));
- The name of the concentration and loading units was changed to g/m^3 and g/m^2 instead of gr/m^3 or gr/m^2;
- The name of the folder fall3d-ver/Utilities/Scripts was changed to fall3d-ver/Utilities/ConfigScripts in order to avoid confusion with fall3d-ver/Scripts created after the compilation of the code.

More information and download at:

- http://bsccase02.bsc.es/projects/fall3d/ or
- http://datasim.ov.ingv.it/Fall3d.html

3 Model equations and parameterizations

The governing equations and the parameterizations used by FALL3D-7.1 are briefly described in the Appendix A "Governing equations and parameterizations". For further details see also Costa et al. (2006); Folch et al. (2009).

4 Overview of I/O files and related programs

FALL3D-7.1 needs the following **input files**:

1) The input file name.inp specifying the control parameters and options. This file is read by FALL3D-7.1 and from all utility programs. An example of name.inp is given in Appendix B.

2) The topography and meteorology database file name.dbs.nc. This file is in NetCDF format and is generated by the pre-process utility program SetDbs (see Section 5.3).

3) The granulometry file name.grn specifying relative fractions and properties of particle classes released from the source. This file is typically generated by the pre-process utility program SetSrc starting from the file name.tgsd describing Total Grain Size Distribution (TGSD), density, and shape of particles. The TGSD file is typically obtained from field data; however it can also be generated by the utility program SetTgsd (see Section 5.2), assuming either a Gaussian or bi-Gaussian distribution (in Φ). A few options are available for the utility program SetSrc to account for aggregation effects on fine ash within the eruptive column (see Section 5.4). In this case an extra aggregation class is added in the name.grn file.

4) The source file name.src specifying the discharge rates at the source points (typically along the eruptive column). This file is generated by the pre-process utility program SetSrc (see Section 5.4).

5) An optional file specifying a list of points (name.pts) where the tracking of some variables is requested (*e.g.* points where to compute tephra arrival times, accumulation rates, etc).

Once a simulation is concluded, FALL3D-7.1 produces the following **output files**:

1) A log file (name.log) containing information about the run (*e.g.*, summary of input data, error and warning messages, etc.)

2) The results file (`name.res.nc`) in NetCDF format (see Appendix C). This file can be processed using several open-source programs (*e.g.* ncview, Panoply, ncl, etc.) to generate plots and animations. Alternatively, the post-process utility program `FALL3D2GMT` (included in the distribution) can be used to generate basic GMT scripts automatically.

3) The tracking points files (`name.tps.*`) containing information about evolution of the variables at the tracked points. Such information is printed as a single output file for each point specified in the input file `name.pts`.

4) A restart file (`name.rst.nc`) in NetCDF format (see Appendix C). This file is used if the restart option is on.

A general flowchart of `FALL3D-7.1` is shown in Figure 1.

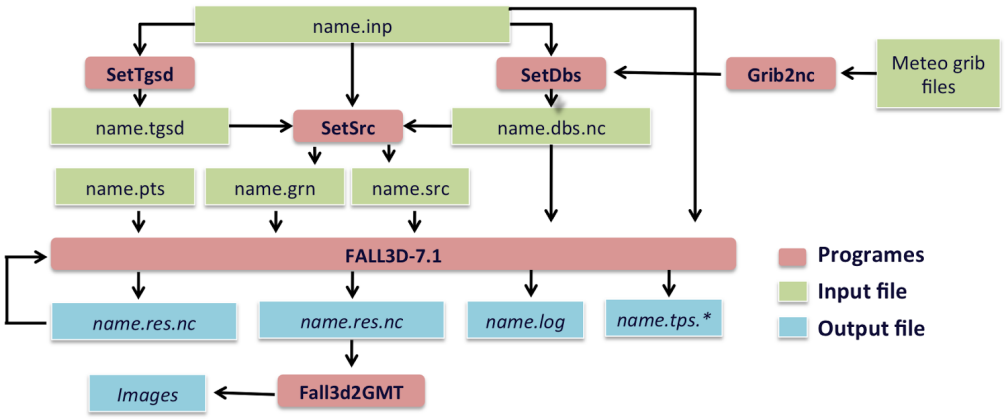

Figure 1: Execution flow of `FALL3D-7.1` and related utility programs. The I/O file names are shown in green/blue.

5 Input files and pre-process utility programs

5.1 The control file `name.inp`

The control input file in ASCII format consists of a set of blocks defining all the computational and physical parameters needed by `FALL3D-7.1` and its related utility programs (`SETTGSD`, `SETDBS`, `SETSRC` and `FALL3D2GMT`). Appendix B shows an example of file `name.inp`. Each program reads only the necessary file blocks generating self-consistent input files. Parameters within a block are listed one per record, in arbitrary order, and optionally can be followed by one (or more) blank space and a comment. The maximum allowed lenght is 256 characters per line including comments. A detailed description of each record is given below. Real numbers can be also expressed using the `FORTRAN` notation (*e.g.*, $12e7 = 12 \times 10^7$).

5.1.1 Block `TIME_UTC`

This block defines variables related to time, such as the period covered by the meteorology file, beginning and end of the eruption, etc. It is used by `FALL3D-7.1` and by the utility programs `SETDBS` and `SETSRC`. The block has the following format:

- `YEAR`: Database starting year (YYYY).

- MONTH: Database starting month (MM).
- DAY: Database starting day (DD).
- BEGIN_METEO_DATA_(HOURS_AFTER_00): Time (in h after 00UTC of the starting day) at which meteorological data start in the database file. This time has to be smaller than time slice defined by the variables: ERUPTION_START_(HOURS_AFTER_00).
- TIME_STEP_METEO_DATA_(MIN): Time step (in min) of the meteorological data in the database file. The time step can be different from that of the original data (*e.g.* if the time step is set at 60 min and the original data were every 6 h, values would be linearly interpolated hourly).
- END_METEO_DATA_(HOURS_AFTER_00): Time slice (in h after 00UTC of the starting day) at which the meteorological data end in the database file. This time has to be larger than time slices defined by the variables: ERUPTION_START_(HOURS_AFTER_00) and RUN_END_(HOURS_AFTER_00) respectively, otherwise the program will stop.
- ERUPTION_START_(HOURS_AFTER_00): Time slice of the eruption start (in h after 00UTC of the starting day). These are nt values ($nt \geq 1$) indicating the starting times of the different eruptive phases. Transient behavior of the eruption column can be described by adding a sufficient number of intervals. Eruptive conditions (plume height, MFR, etc.) are assumed constant during each phase. The first value must be equal or larger than the value of the record BEGIN_METEO_DATA_(HOURS_AFTER_00).
- ERUPTION_END_(HOURS_AFTER_00): Time slice of the eruption end (in h after 00UTC of the starting day). This is the time slice at which the source term is switched off (*i.e.* the time at which the last eruptive phase ends).
- RUN_END_(HOURS_AFTER_00): Time slice of the run (in h after 00UTC of the starting day). This value has to be equal or smaller than the value of the variable END_METEO_DATA_(HOURS_AFTER_00). Note that, in general, a run should continue even after the source term is switched off (*i.e.* when the eruption has stopped) in order to allow the remaining airborne particles to sediment completely.
- RESTART: If YES, the run starts from the restart file name.rst.nc generated at the end of a previous run.

5.1.2 Block GRID

This block defines the grid variables needed by SETDBS and FALL3D-7.1. The block has the following format:

- COORDINATES: Map projection options. The two available options are LON-LAT (accounting for Earth's curvature) or UTM. It is recommended to use LON-LAT (from version 7.1 the option UTM is advised not to be used, although still available for backwards compatibility). The UTM option can only be used if the domain is within a unique UTM zone. The use of the UTM coordinate system in large domains covering more than one UTM zone is not allowed. The sub-blocks LON_LAT or UTM are read in each case respectively.
- LONMIN: Minimum longitude (in decimal degrees) of the domain (*i.e.* longitude corresponding to the bottom left corner). Only used in the LON-LAT option.
- LONMAX: Maximin longitude (in decimal degrees) of the domain (*i.e.* longitude corresponding to top right corner). Only used in the LON-LAT option.
- LATMIN: Minimum latitude (in decimal degrees) of the domain (*i.e.* latitude corresponding to bottom left corner). Only used in the LON-LAT option.
- LATMAX: Maximin latitude (in decimal degrees) of the domain (*i.e.* latitude corresponding to top right corner). Only used in the LON-LAT option.

- `LON_VENT`: Vent longitude. Only used in the LON-LAT option.
- `LAT_VENT`: Vent latitude. Only used in the LON-LAT option.
- `UTMZONE`: UTM zone code in format nnL (*e.g.* 33S). Only used in the UTM option.
- `XMIN`: minimum x-coordinate of the domain (bottom left corner). UTM coordinates must be given in m. Only used in the UTM option.
- `XMAX`: maximum x-coordinate of the domain (top right corner). UTM coordinates must be given in m. Only used in the UTM option.
- `YMIN`: minimum y-coordinate of the domain (bottom left corner). UTM coordinates must be given in m. Only used in the UTM option.
- `YMAX`: maximum y-coordinate of the domain (top right corner). UTM coordinates must be given in m. Only used in the UTM option.
- `X_VENT`: x-coordinate of the vent. UTM coordinates must be given in m. Only used in the UTM option.
- `Y_VENT`: y-coordinate of the vent. UTM coordinates must be given in m. Only used in the UTM option.
- `VENT_HEIGHT`: Height of the vent a.s.l. (in m).
- `NX`: Number of grid nodes in the x-direction.
- `NY`: Number of grid nodes in the y-direction.
- `ZLAYER_(M)`: Array of heights (in m) of the vertical z-layers in terrain following coordinates. The vertical layers can be specified manually (as an array of values) or, for equally spaced vertical discretization, simply indicating the limits and the increment (*e.g.* `FROM 0 TO 10000 INCREMENT 1000`). It is not necessary to specify the number of vertical layers since it is automatically calculated.

5.1.3 Block `GRANULOMETRY`

This block defines the variables needed by the `SETTGSD` utility program to generate the TGSD file `name.tgsd`. The block has the following structure:

- `DISTRIBUTION`: Type of distribution. The two available TGSD are: `GAUSSIAN` or `BIGAUSSIAN`, where Gaussian or bi-Gaussian distribution is referred to a Gaussian or bi-Gaussian distribution in Φ, where $\Phi = \log_2 d(\text{in mm})$.
- `NUMBER_OF_CLASSES`: Number of granulometric classes in the TGSD. Note that this value can be different from the number of classes in `FALL3D-7.1` (aggregate class and/or volatiles can be added later in the granulometry file `name.grn`, created by `SETSRC`).
- `FI_MEAN`: Mode of Gaussian distribution in Φ. For Bi-Gaussian distributions two values must be provided.
- `FI_DISP`: Standard deviation (σ) of the Gaussian distribution in Φ. For Bi-Gaussian distributions two values must be provided.
- `FI_RANGE`: Minimum and maximum values for the range of Φ considered (Φ_{min} and Φ_{max} respectively).
- `DENSITY_RANGE`: Values of densities ρ_{min} and ρ_{max} (in kg/m^3) associated to $\Phi = -1$ and $\Phi = 6$ for coarse and fine pumices respectively (e.g Bonadonna and Phillips, 2003). Linear interpolation is assumed between these two extremes and constant beyond them. In particular, if $\rho_{min} = \rho_{max}$, density will be constant for all classes.

- SPHERICITY_RANGE: Values of sphericity ψ_{min} and ψ_{max} associated to Φ_{min} and Φ_{max} particles. Linear interpolation is assumed between these two extremes and constant beyond them. In particular, if $\psi_{min} = \psi_{max}$, sphericity is constant for all classes.
- MIXING_FACTOR: Only read if distribution type is BIGAUSSIAN. Relative weight p of grain-size sub-populations, i.e. p for the coarse sub-population and $1 - p$ for the fine sub-population. If this parameter is not specified is set to its default value of 0.5.

5.1.4 Block SOURCE

This block defines the variables needed by the SETSRC utility program to generate the source term (eruptive column) for each of the $nt \geq 1$ eruptive phases. The block has the following format:

- SOURCE_TYPE: Type of source distribution. The available options are POINT, SUZUKI, PLUME or RESUSPENSION.

1) In the case SOURCE_TYPE = POINT only the sub-block POINT_SOURCE is used:

- MASS_FLOW_RATE_(KGS): Array of values of the mass flow rate (in kg/s) for the nt eruptive phases. Alternatively, the user can choose among the options ESTIMATE-MASTIN (Mastin et al., 2009), ESTIMATE-DEGRUYTER (Degruyter and Bonadonna, 2012) or ESTIMATE-WOODHOUSE (Woodhouse et al., 2013) and SETSRC automatically computes the MFR from the column heights based on empirical fits. The last two options account for cross wind effects on plume height and MFR.
- HEIGHT_ABOVE_VENT_(M): Array of column heights (in m above the vent) for the nt eruptive phases. Note that the plume heights must be lower than the top of the computational domain, specified in the variable ZLAYER_(M) of the GRID block. Otherwise, the program will stop.

2) In the case SOURCE_TYPE = SUZUKI only the sub-block SUZUKI_SOURCE is used:

- MASS_FLOW_RATE_(KGS): Array of values of the mass flow rate (in kg/s) for the nt eruptive phases. Alternatively, the user can choose among the options ESTIMATE-MASTIN (Mastin et al., 2009), ESTIMATE-DEGRUYTER (Degruyter and Bonadonna, 2012) or ESTIMATE-WOODHOUSE (Woodhouse et al., 2013) and SETSRC automatically computes the MFR from the column heights based on empirical fits. The last two options account for cross wind effects on plume height and MFR.
- HEIGHT_ABOVE_VENT_(M): Array of column heights (in m above the vent) for the nt eruptive phases. Note that the plume heights must be lower than the top of the computational domain, specified in the record ZLAYER_(M) of the GRID block. If not, the program will stop.
- A: Array of values of the parameter A in the Suzuki distribution (Pfeiffer et al., 2005) for the nt eruptive phases.
- L: Array of values of the parameter λ in the Suzuki distribution (Pfeiffer et al., 2005) for the nt eruptive phases.

3) In the case SOURCE_TYPE = PLUME only the sub-block PLUME_SOURCE is used:

- SOLVE_PLUME_FOR: The two available options are MFR or HEIGHT. In the first case SETSRC solves for the mass flow rate given the column height, whereas in the second does the opposite.
- MFR_SEARCH_RANGE: Two values n and m such that 10^n and 10^m specify the range of MFR values admitted in the iterative solving procedure (*i.e.* it is assumed that $10^n \leq MFR \leq 10^m$). Only used if SOLVE_PLUME_FOR=MFR.
- MASS_FLOW_RATE_(KGS): Values of the mass flow rate (in kg/s) for the nt eruptive phases. Only used if SOLVE_PLUME_FOR=HEIGHT.
- HEIGHT_ABOVE_VENT_(M): Heights of the plume (in m above the vent) for the nt eruptive phases. Note that the plume heights must be lower than the top of the computational domain, specified in the variable ZLAYER_(M) of the GRID block. Only used if SOLVE_PLUME_FOR=MFR.

- EXIT_VELOCIY_(MS): Values of the magma exit velocity (in m/s) at the vent for the nt eruptive phases.
- EXIT_TEMPERATURE_(K): Values of the magma exit temperature (in K) at the vent for the nt eruptive phases.
- EXIT_WATER_FRACTION_(IN%): Values of the magma volatile fraction (in weight percent) at the vent for the nt eruptive phases.

4) In the case SOURCE_TYPE = RESUSPENSION only the sub-block RESUSPENSION is used:

- MAX_RESUSPENSION_SIZE_(MIC) : Maximum particle size (in μm) for which resuspension is allowed. This is typically few hundreds of μm.
- DEPOSIT_THRESHOLD_(KGM2) : Value of the deposit load (in kg/m^2) encompassing the area where resuspension is considered. This is used to prevent resuspension in areas with negligible original deposit loads.
- MAX_INJECTION_HEIGHT_(M): Maximum height of resuspension (in m). Resuspended ash is uniformly distributed vertically from the ground level to this maximum height.
- EMISSION_SCHEME: Type of ash emission scheme (see Appendix A "Governing equations and parameterizations" for further details). The available options are WESTPHAL (based on Westphal et al., 1987), MARTICORENA (based on Marticorena and Bergametti, 1995; Marticorena et al., 1997) or SHAO (based on Shao et al., 1993; Shao and Leslie, 1997; Shao and Lu, 2000).
- EMISSION_FACTOR: Tuning factor of the emission scheme.
- THRESHOLD_UST: Value of the threshold friction velocity. Only used if EMISSION_SCHEME = WESTPHAL
- MOISTURE_CORRECTION: If YES, threshold friction velocity is corrected for soil moisture according to Fecan et al. (1999).

5.1.5 Block AGGREGATION

This block defines the variables needed by SETSRC program in order to modify the original TGSD to account for ash aggregation effects. It is assumed that one aggregated class is formed. The block has the following format:

- AGGREGATION_MODEL: Aggregation parameterization. Available options are NONE, PERCENTAGE (based on Sulpizio et al., 2012), CORNELL (based on Cornell et al., 1983) or COSTA (based on Costa et al., 2010, to be used with the option PLUME only).
- FI_AGGREGATES: $\Phi-$class of aggregates (i.e. main mode).
- DENSITY_AGGREGATES: Density of aggregates.
- VSET_FACTOR: Multiplicative correction factor for settling velocity of aggregates.
- PERCENTAGE_(%): Percentage of ash aggregating for classes <FI_AGGREGATES.
  Only read if AGGREGATION_MODEL = PERCENTAGE
- FRACTAL_EXPONENT: Fractal exponent (see Costa et al., 2010, for details).
  Only read if AGGREGATION_MODEL = COSTA

5.1.6 Block AEROSOLS

This block defines the variables needed by SETSRC program in order to add aerosol tracers. This block defines whether aerosol (indicated as SO_2) is transported or not and in which percentage (in wt %). In FALL3D-7.1 only passive transport is considered, *i.e.* SO_2 here is simply considered a tracer and can be used to simulate the transport of any passive volatile. It is expected to add chemical reactions in future code releases. The block has the following format:

- SO2: Defines whether SO_2 transport is switched on or off. Options are YES (on) or NO (off).
- PERCENTAGE_(%): Percentage of SO_2 with respect to the total mass.

Note that water is however transported as an additional class when SOURCE_TYPE = PLUME consistently with the water fraction specified in EXIT_WATER_FRACTION_(IN%) in the block SOURCE whereas, for computational simplicity, the mass of the aerosol *i.e.* SO_2 (however typically smaller than a few %) is added to the total mass, i.e. mass fraction considering SO_2 is not normalized.

5.1.7 Block GRAVITY_CURRENT

This block defines the variables needed by FALL3D-7.1 in order to describe the effect of volcanic cloud spreading as a gravity current at the NBL. The model is based on Woods and Kienle (1994); Sparks et al. (1997) and parameter estimations by Suzuki and Koyaguchi (2009). The block has the following format:

- GRAVITY_CURRENT: Defines whether the gravity current model is switched on or off.
  The available options are YES (on) or NO (off).
- C_FLOW_RATE: Empirical constant for volumetric flow rate at NBL.
  Read only if GRAVITY_CURRENT = YES.
- LAMBDA_GRAV: Empirical constant for the gravity current model.
  Read only if GRAVITY_CURRENT = YES.
- K_ENTRAIN: Entrainment coefficient for the gravity current model.
  Read only if GRAVITY_CURRENT = YES.
- BRUNT_VAISALA: Frequency of Brunt–Vaisala due to the ambient stratification.
  Read only if GRAVITY_CURRENT = YES.

5.1.8 Block FALL3D

This block defines the specific variables related to physics in the FALL3D-7.1 program. The block has the following format:

- TERMINAL_VELOCITY_MODEL: Type of terminal settling velocity model. The available options are ARASTOOPOUR, GANSER, WILSON, and DELLINO.
- VERTICAL_TURBULENCE_MODEL: Type of model for vertical diffusion. The available options are CONSTANT or SIMILARITY.
- VERTICAL_DIFFUSION_COEFFICIENT_(M2/S): Value of the diffusion coefficient (in m^2/s). Only used if VERTICAL_TURBULENCE_MODEL = CONSTANT
- HORIZONTAL_TURBULENCE_MODEL: Type of model for horizontal diffusion. The available options are CONSTANT, RAMS, or CMAQ.
- HORIZONTAL_DIFFUSION_COEFFICIENT_(M2/S): Value of the diffusion coefficient (in m^2/s). Only used if HORIZONTAL_TURBULENCE_MODEL = CONSTANT.
- RAMS_CS: Value of C_S in the RAMS model (see eq. 6). Only used if HORIZONTAL_TURBULENCE_MODEL = RAMS.
- WET_DEPOSITION: Defines whether wet deposition model based on precipation rate is switched on or off. Options are YES (on) or NO (off).

5.1.9 Block OUTPUT

This block defines specific variables related to output strategy in the FALL3D-7.1 program. The block has the following structure:

- POSTPROCESS_TIME_INTERVAL_(HOURS): Postprocess time interval in hours.
- POSTPROCESS_3D_VARIABLES: The available options are YES or NO. If YES, FALL3D-7.1 writes 3D concentration in the output file filename.res.nc. If NO, only 2D variables are written to the output file (this can be desirable for very large files).
- POSTPROCESS_CLASSES: The available options are YES or NO. If YES, FALL3D-7.1 writes results for all classes. If NO, only total results are written. Take into account that the size of the FALL3D-7.1 output file is directly proportional to the number of classes.
- TRACK_POINTS: The available options are YES or NO. If YES, FALL3D-7.1 writes the tracking points files defined in the input file name.pts.

5.1.10 Block POSTPROCESS

This block of data is read by the post-process utility program FALL3D2GMT, which writes a script used to post-process results using GMT. The block has the following format:

- CROP_DOMAIN: Values for LONMIN, LONMAX, LATMIN, and LATMIN of the GMT domain. Note than the domain in GMT (domain of the plot) can be smaller than the simulation domain.
- MAP_TOPOGRAPHY: The available options are YES or NO. If YES, FALL3D2GMT plots topography contours (in m) as specified in the corresponding CONTOUR_LEVELS line.
- MAP_TOTAL_LOAD: The available options are YES or NO. If YES, FALL3D2GMT plots contours of total deposition load (in kg/m^2) as specified in the corresponding CONTOUR_LEVELS line.
- MAP_WET_LOAD: The available options are YES or NO. If YES, FALL3D2GMT plots contours of total wet deposition load (in kg/m^2) as specified in the corresponding CONTOUR_LEVELS line. Note that this is possible only when WET_DEPOSITION is set to YES.
- MAP_CLASS_LOAD: The available options are YES or NO. If YES, FALL3D2GMT plots contours of class deposition load (in kg/m^2) as specified in the corresponding CONTOUR_LEVELS line. Note that this is possible only when POSTPROCESS_CLASSES is set to YES.
- MAP_CLASS_WET: The available options are YES or NO. If YES, FALL3D2GMT plots contours of class wet deposition load (in kg/m^2) as specified in the corresponding CONTOUR_LEVELS line. Note that this is possible only when WET_DEPOSITION and POSTPROCESS_CLASSES are set to YES.
- MAP_DEPOSIT_THICKNESS: The available options are YES or NO. If YES, FALL3D2GMT plots contours of total deposit thickness converted using the density value specified in the DEPOSIT_DENSITY_(KG/M3) line (by default set to 1000). Values can be expressed in mm, cm, or m in accord to the UNITS line for the contours specified in the corresponding CONTOUR_LEVELS line.
- MAP_CONCE_GROUND: The available options are YES or NO. If YES, FALL3D2GMT plots contours of total concentration at ground level (in g/m^3) as specified in the corresponding CONTOUR_LEVELS line.
- MAP_PMxx_GROUND: The available options are YES or NO. If YES, FALL3D2GMT plots contours of PM_5, PM_{10}, and PM_{20} concentrations at ground level (in g/m^3) as specified in the corresponding CONTOUR_LEVELS line.
- MAP_COLUMN_MASS: The available options are YES or NO. If YES, FALL3D2GMT plots contours of total column mass (in g/m^2) as specified in the corresponding CONTOUR_LEVELS line.

- MAP_COLUMN_PMxx: The available options are YES or NO. If YES, FALL3D2GMT plots contours of PM_5, PM_{10}, and PM_{20} column mass (in g/m^2) as specified in the corresponding CONTOUR_LEVELS line. These are useful quantities to compare with satellite imagery.
- MAP_FLIGHT_LEVEL:The available options are YES or NO. If YES, FALL3D2GMT plots contours of concentration at different Flight Levels (in g/m^3) as specified in the corresponding CONTOUR_LEVELS line. By default, these are FL050, FL100, FL150, FL200, FL250, FL300, FL350 and FL400. However, the number and values of the different FL can be easily modified (just edit the FALL3D-7.1 source file InpOut.f90, modify nflevel as desired and re-complie the code).
- MAP_AOD: The available options are YES or NO. If YES, FALL3D2GMT plots contours Aerosol Optical Depth as specified in the corresponding CONTOUR_LEVELS line.

5.2 The TGSD file name.tgsd

The TGSD file is an ASCII file containing the definition of the particle classes (a class is characterized by particle size, density and sphericity) without aggregates nor aerosol components. Note that in the previous versions of the code this file was called name.grn. The file format is described in Table 1 and the meaning of the used symbols is the following:

- nc: Number of particle classes.
- diam: Class diameter (in mm).
- rho: Class density (in kg/m^3).
- sphe: Class sphericity.
- fc: Class mass fraction (0-1). It must verify that $\sum$ fc = 1.

nc
diam(1) rho(1) sphe(1) fc(1)
...
diam(nc) rho(nc) sphe(1) fc(nc)

Table 1: Format of the TGSD file name.tgsd.

5.2.1 The utility program SETTGSD

The utility program SETTGSD can be used to generate the TGSD file name.tgsd in accordance with the parameters specified in the block GRANULOMETRY of the input file name.inp. This program generates only Gaussian and Bi-Gaussian distributions in Φ (log-normal in d) and assumes a linear increase of density ρ and sphericity ψ between the two extremes specified by the user. For other grain size distributions, the user must provide the TGSD file (typically derived from field data). Note that in the previous versions of the code this utility program was called SETGRN.

5.3 The meteorological database file name.dbs.nc

The file name.dbs.nc, written in NetCDF format (see Appendix C), contains topography and time-dependent meteorological data needed by FALL3D-7.1 (wind field, air temperature and density, humidity, etc), written in terrain-following coordinates. The file is created by the utility program SETDBS, which interpolates meteorological data from the original grid of meteorological models to the FALL3D-7.1 computational domain. In turn, SETDBS requires a specific naming convention for the original NetCDF meteorological data. For this reason, another utility program (GRIB2NC) can be used in combination with wgrib/wgrib2 to decode and convert original grib-format meteorological data to the required NetCDF format. There are a several options to generate this database file depending on the scale of application.

Model	Native data format	need of GRIB2NC
Global model forecasts		
GFS at 1^o resolution	grib	yes
GFS at 0.5^o resolution	grib	yes
Global analysis and re-analysis		
NCEP final analysis at 1^o resolution	grib	yes
NCEP re-analysis 1	grib	no
NCEP re-analysis 2	grib	no
ECMWF ERA-40 re-analysis	grib	yes
ECMWF ERA-Interim re-analysis	grib	yes
Mesoscale models		
WRF-ARW	NetCDF	no
ETA	grib	yes
ARPA-SIM	grib	yes
Others (local-scale options)		
CALMET-6.2	own-binary	no
Vertical profile	ASCII	no

Table 2: List of different options handled by the SETDBS pre-process utility program. Native data in grib format needs to be converted first to NetCDF using the GRIB2NC program before running SETDBS.

5.3.1 The utility program SETDBS

The pre-process utility program SETDBS generates the database file name.dbs.nc in accordance with the parameters specified in the blocks TIME_UTC and GRID of the input file name.inp. After running the utility GRIB2NC , the program SETDBS can use meteorological data from different independent meteorological models and interpolates variables onto the FALL3D-7.1 computational grid. The time duration of the database must be equal or larger than the duration of the simulation. The possible options are listed in Table 2 and described below.

- The simplest option consists of using a horizontally uniform wind derived from a single vertical profile, typically obtained from sounding measurements or from indirect reconstructions. The vertical profile needs to be specified in the ASCII file name.profile using the format described in the Appendix D. In this case, in addition to the profile name.profile it is also necessary to furnish a topography file name.top in GRD format (see Appendix E). It is recommended to use this very simplistic option (homogeneous wind field) only when no other meteorological data are available.
- The second choice (CALMET option) uses data derived from the output of the meteorological diagnostic model CALMET (Scire et al., 2000). This option is typically used for assimilating and interpolating short-term forecasts (or re-analysis) from Mesoscale Meteorological Prognostic Models (MMPM) to a finer scale. In this case only the UTM coordinate system can be used. Note that the output of CALMET is a binary file that depends on the architecture of the machine where it was generated. Moreover note that this option is compatible only with a CALMET output time step equal to an hour (*i.e.*, nsecdt=3600).
- The third choice (strongly recommended) uses data from global/mesoscale forecasts or analysis/re-analysis. Global data (assumed to be downloaded in grib format) have to be decoded and converted to NetCDF using the utility program GRIB2NC before running SETDBS.

5.3.2 The utility program GRIB2NC

The utility program GRIB2NC runs in combination with wgrib/wgrib2 and dedicated scripts (see Section 7.7) in order to convert grib format data to a NetCDF file readable by SETDBS. Possible options are:

1. GFS forecasts at 1^o and 0.5^o resolution.

- http://nomad3.ncep.noaa.gov/ncep_data/index.html
- http://www.nco.ncep.noaa.gov/pmb/products/gfs
- 26 pressure levels starting at 10 mb (10 20 30 50 70 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 925 950 975 1000).
- 7 days ahead (00 cycle assumed).

2. NCEP GFS final analysis (FNL) at 1^o resolution. This product is from the Global Data Assimilation System (GDAS). The FNLs are made with the same model which NCEP uses in the Global Forecast System (GFS), but the FNLs are prepared about an hour or so after the GFS is initialized.
   - http://rda.ucar.edu/datasets/ds083.2/
   - 26 pressure levels starting at 10 mb (10 20 30 50 70 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 925 950 975 1000).
   - 4-times daily.
   - Temporal range: 30 July 1999 to present.
3. CDAS-NCEP/NCAR reanalysis 1 at 2.5^o resolution.
   - http://nomad3.ncep.noaa.gov/ncep_data/index.html
   - 17 pressure levels starting at 10 mb (10 20 30 50 70 100 150 200 250 300 400 500 600 700 850 925 1000).
   - 4-times daily.
   - Temporal range: 1 January 1948 to present.
   - NOTE: only pressure levels 00 cycle grib files (pgb.ft00.YYYYMM) are used.
4. NCEP Reanalysis 2 at 2.5^o resolution.
   - http://nomad3.ncep.noaa.gov/ncep_data/index.html
   - 17 pressure levels starting at 10 mb (10 20 30 50 70 100 150 200 250 300 400 500 600 700 850 925 1000).
   - 4-times daily.
   - Temporal range: 1 January 1979 to present.
   - NOTE: only pressure levels grib files (pgb.YYYYMM) are used.
5. ECMWF ERA-40 reanalysis.
   - http://apps.ecmwf.int/datasets/data/era40_daily
   - 23 pressure levels starting at 1 mb (1 2 3 5 7 10 20 30 50 70 100 150 200 250 300 400 500 600 700 775 850 925 1000).
   - 4-times daily.
   - Temporal range: 1 September 1957 to 31 August 2002.
   - NOTE 1: Files are downloaded separately for pressure, non-pressure (surface) and invariant variables. Required variables are: i) pressure: Geopotential, Relative humidity, Temperature, U component of wind, V component of wind, Vertical velocity, ii) Surface: 10 metre U wind component, 10 metre V wind component, 2 metre temperature, Boundary layer height, iii) Invariant: Geopotential, Land-sea mask. Variable files must be named with standard ECMWF names, i.e. `hgt.grib, temp.grib, rhum.grib, omega.grib, uvel.grib, vvel.grib, t2sfc.grib, u10sfc.grib, v10sfc.grib,`.
   - NOTE 2: Downloading a domain subset with different resolutions (lower than 0.25^o) is possible.
6. ECMWF ERA-Interim reanalysis.

- http://apps.ecmwf.int/datasets/data/interim_full_daily
- 37 pressure levels starting at 1 mb (1 2 3 5 7 10 20 30 50 70 100 125 150 175 200 225 250 300 350 400 450 500 550 600 650 700 750 775 800 825 850 875 900 925 950 975 1000).
- 4-times daily.
- Temporal range: 1 January 1979 to present.
- NOTE 1: Files are downoladed separately for pressure, non-pressure (surface) and invariant variables. Required variables are: i) pressure: Geopotential, Relative humidity, Temperature, U component of wind, V component of wind, Vertical velocity, ii) Surface: 10 metre U wind component, 10 metre V wind component, 2 metre temperature, Boundary layer height, iii) Invariant: Geopotential, Land-sea mask.
- NOTE 2: Downloading a domain subset with different resolutions (lower than 0.25^o) is possible.

5.4 The source file `name.src`

The source file `name.src` is an ASCII file containing the definition of the source term. The source can be defined for different time phases during which source values are kept constant. The number, position and values (*i.e.* Mass Flow Rate) of the source points can vary from one time slice to another and cannot overlap. There is no restriction on the number and duration of the time slices. It allows, in practice, to discretize any kind of source term. This file can be defined directly by the user or generated by the pre-process utility program `SETSRC`. The format of the file `name.src` is described in Table 3 and the meaning of the used symbols is the following:

- `itime1`: Source starting time (in sec after 00UTC of the eruption starting day).
- `itime2`: End time (in sec after 00UTC of the eruption starting day).
- `nsrc`: Number of source points (it can vary from one interval to another depending on the column height).
- `nc`: Total number of particle classes (as in the file `name.grn`).
- `MFR`: Mass flow rate (in kg/s).
- `x`: Longitude or x-coordinate of the source $isrc$.
- `y`: Latitude or y-coordinate of the source $isrc$.
- `z`: z-coordinate of the source point above ground level (a.g.l.) (in m).
- `i`,`j`,`k`: indexes of the source point in the `FALL3D-7.1` mesh.
- `src`: Mass flow rate (in kg/s) of each granulometric class for this point source. It must be verified that $\sum\sum src(isrc, ic) = MFR$.

itime1 itime2
nsrc nc
MFR
x y z i j k src(1,1) ... src(1,nc)
...
x y z i j k src(nsrc,1) ... src(nsrc,nc)

Table 3: Format of the source file `name.src`. This block is repeated for each eruption phase.

5.4.1 The utility program SETSRC

The utility program SETSRC is used to generate 1) the source file name.src in accordance with the parameters specified in the blocks TIME_UTC and SOURCE of the input file name.inp and 2) modify the preliminary TGSD file name.tgsd in order to create the granulometry file name.grn used by FALL3D-7.1 and consistent with the aggregation and aerosol options specified in the blocks AGGREGATION and AEROSOLS of the control file name.inp.
Available options are *i*) a point source column, *ii*) a mushroom-like shape column (Suzuki option), *iii*) an eruption column model based on the Buoyant Plume Theory (BPT) or *iv*) a diffuse emission for ash resuspension.

5.5 The granulometry file name.grn

The granulometry file is an ASCII file containing the characterization of the particle classes and, optionally, aggregates and aerosols. This file is created by the utility program SETSRC from the preliminary TGSD file name.tgsd. Note that this file is different from the one used in the previous versions of the code. The file format is described in Table 4 and the meaning of the used symbols is the following:

- nc: Total number of particle classes (differs from nc in the TGSD file in case of aggregation or aerosols).
- diam: Class diameter (in mm).
- rho: Class density (in kg/m^3).
- sphe: Class sphericity.
- fc: Class mass fraction (0-1). It must verify that $\sum$ fc = 1.
- class: Label denoting class (particle/gas typology) such particle class, aggregate or gas.

nc				
diam(1)	rho(1)	sphe(1)	fc(1)	class(1) (*e.g. class-01*)
...	...	...	...	...
diam(nc-2)	rho(nc-2)	sphe(nc-2)	fc(nc-2)	class(nc-2) (*e.g. aggregate*)
diam(nc-1)	rho(nc-1)	sphe(nc-1)	fc(nc-1)	class(nc-2) (*e.g. H2O*)
diam(nc)	rho(nc)	sphe(nc)	fc(nc)	class(nc-2) (*e.g. SO2*)

Table 4: Format of the granulometry file name.grn

Note that when the option COSTA is selected as the aggregation model, the variable fc is automatically calculated by setsrc since it can vary with time.

5.6 The tracking points file name.pts

This file contains the names (identifiers) and coordinates of the points to be tracked. It is used only when the record TRACK_POINTS in the input file name.inp is set to YES. The format of the file name.pts consists of lines (one line per point) with three columns specifying the point name, the point longitude (or x-coordinate if UTM coordinates are used), and the point latitude (or y-coordinate if UTM coordinates are used). If available, an extra column with measurements of tephra loading on the ground can be added for a sake of comparison with simulation results. There is no limit on the number of points to track. The file format is described in Table 5.

location-1	x-coord-1	x-coord-1	measurement-1
location-2	x-coord-2	x-coord-2	measurement-2
location-3	x-coord-3	x-coord-3	measurement-3
location-4	x-coord-4	x-coord-4	measurement-4
...	...	...	...
location-n	x-coord-n	x-coord-n	measurement-n

Table 5: Format of the granulometry file `name.pts`

6 Output files and post-process utility programs

6.1 The log file `name.log`

The file `name.log` is an ASCII file where critical information about the simulation run is stored. The information written on the `name.log` contains:

- `FALL3D-7.1` copyright;
- code version;
- number of processors;
- starting time of the simulation;
- input files names and paths;
- output files names and paths;
- time range and grid data of the meteorological database;
- `FALL3D-7.1` input data (*e.g.* time range; numerical parameters; output options; etc);
- memory requirements;
- source terms features;
- particle classes;
- atmospheric properties, horizontal, and vertical diffusion;
- terminal velocities;
- main parameters of the gravity current model;
- updates about the simulation such as iteration number, critical time step, elapsed time, current (simulation time), and a mass balance for the total mass (inside and ouside the computational domain) and the erupted mass.

6.2 The results file `name.res.nc`

This file, written in netCDF format, contains the following output variables:

- particle properties (diameter, density and sphericity);
- topography;
- ground load and, if specified in the control input file, class ground load;
- wet deposition and, if specified in the control input file, class wet deposition;
- deposit thickness;

- total and PM_{xx} (xx=5, 10, 20) concentration at ground level;
- total and PM_{xx} (xx=5, 10, 20) column mas load (vertical integration of concentration);
- concentration at different flight levels. By default, these are FL050, FL100, FL150, FL200, FL250, FL300, FL350, and FL400. However, these values can be reconfigured by modifying the InpOut.f90 source file and recompiling the code;
- aerosol optical depth;
- total and class concentration at all model layers (if specified in the control input file only).

6.3 The restart file `name.rst.nc`

The restart file, written in netCDF format, can be used to start a new run from the end of a previous simulation. The file is automatically created each time `FALL3D-7.1` prints its results. If `RESTART = YES` in the block `TIME_UTC` of `name.inp`, a run is initialized with the airborne concentration specified in the restart file `name.rst.nc`. Any restart file previously created is destroyed whenever a new restart file is printed.

7 Program installation and execution

IMPORTANT NOTE: Please read very carefully all this section before installing and running `FALL3D-7.1`.

7.1 Pre-Installation requirements

`FALL3D-7.1` is written in `FORTRAN-90` and requires the external library netCDF. The code has been tested in UNIX/Linux platforms including MacOS X. The source code can be compiled to run in serial mode (one processor) and parallel mode (multiple processor and/or clusters based on MPI). For compiling the serial version you will need:

- A Fortran 90 compiler (eg: ifort, gfortran, xlf90, etc.)
- The Library netCDF installed on your machine (versions 3.6.*, 4.* or later). NetCDF library is available from: http://www.unidata.ucar.edu/netcdf/

In addition, for compiling the parallel version (optional), you will need:

- MPI or OpenMPI installed on you machine with Fortran compilation enabled (command `mpif90` must be available on your machine).

To decode meteorological data in grib format (see Table2) using `GRIB2NC` you will need:

- `wgrib` and/or `wgrib2`, available from http://www.cpc.ncep.noaa.gov/products/wesley/wgrib.html

Finally, if you wish to use post-process results using the utility program `FALL3D2GMT` (optional) you will need:

- The Generic Mapping Tools (GMT) library, available from http://gmt.soest.hawaii.edu/projects/gmt/wiki/Download

7.2 Installation

Sources of `FALL3D-7.1` are distributed as a gzipped tar archive in a file named `fall3d-7.1.tar.gz`, available at the following URLs:

`http://bsccase02.bsc.es/projects/fall3d/`
`http://datasim.ov.ingv.it/Fall3d.html`

After you obtained file `fall3d-7.1.tar.gz`, copy it in a directory (eg: your home directory) and unpack the tarball with the command:

```
$ tar zxvf fall3d-7.1.tar.gz
```

This creates the installation directory tree with the root directory named `fall3d-7.1`. The directory tree is shown in Table 6.

Table 6: Default structure of `fall3d-7.1` sub-folders.

```
Manual                        # Contains this manual
Example                       # Contains an example of input file (name.inp)
libMaster                     # Master library for Fall3d and utilities
Utilities                     # Utilities root directory
Utilities/Grib2nc             # Grib2nc sources
Utilities/Grib2nc/config      # Grib2nc sample configuration files
Utilities/SetTgsd             # SetTgsd sources
Utilities/SetDbs              # SetDbs sources
Utilities/ConfigScripts       # Shell script sources
Utilities/Fall3d2GMT          # Fall3d2GMT sources
Utilities/SetSrc              # SetSrc sources
Scripts                       # This is generated by './configure'
bin                           # This is generated by 'make install'
```

The package comes with a `configure` script for automatically configuring your installation.

The '`configure`' shell script attempts to guess correct values for various system-dependent variables used during compilation. Then uses these values to create a '`Makefile`' in each directory of the package for compiling and installing the code and the scripts.

The configuration script does not automatically set the compiler flags. It is strongly suggested to set the compiler optimization flag "-O" by setting the environmental variable FCFLAGS=-O or by setting it in the `configure` command line, as shown below.

In brief, to configure, compile and install `FALL3D-7.1` (serial version) it should be enough to issue the following commands:

```
$ cd fall3d-7.1
$ ./configure FCFLAGS=-O
$ make
$ make install
```

For installing both the serial and the parallel versions the commands are:

```
$ cd fall3d-7.1
$ ./configure FCFLAGS=-O --enable-parallel
$ make
$ make install
```

By default, the binary files are installed in the directory '`bin`' and the shell scripts (used to launch `FALL3D-7.1` and all the related utility programs) in the directory '`Scripts`', both under the root directory `fall3d-7.1`. Please note that the shell scripts located in directory '`Scripts`' are generated by '`configure`' and contain pointers to the location of the binaries. The shell scripts can be moved/copied to other directories, but the binary files must be left in the '`bin`' directory. The default location of the `bin` directory can be changed by providing proper flags to the '`configure`' script, as described below (see flag `--prefix` or `--exec-prefix`). In the default configuration, the wind data are searched in the directory '`$HOME/Data`' and the `FALL3D-7.1` runs are stored in the directory '`$HOME/Runs`'. However, these directories can be modified as described below. In this version of `Fall3d`, the variable `SCRIPTDIR`, cannot be changed; however the directory `$SCRIPTDIR` can be moved to another location after the installation.

7.3 Multiple installations

Multiple installations of FALL3D-7.1 on the same system might be needed. This is usually the case when a disk is shared among different computer platforms and/or when you want different versions of FALL3D-7.1 compiled for different platforms or on a single platform but with different libraries and compilers. To do this, just untar file '`fall3d-7.1.tar.gz`' into different directories and configure each replica of FALL3D-7.1 using different configuration flags. In this case, the binaries may reside in different directories, but can share the same data file (eg: the same '`DATADIR`' and '`RUNDIR`' directories). The different binaries can be launched by the corresponding shell scripts (located in the corresponding directory '`SCRIPTDIR`').

7.4 Customizing the installation

You may choose different configuration parameters, including the fortran compiler, compilation flags, the netCDF version (if you have more than one) and the location of the directories '`bin`', `Scripts`', '`Data`' and '`Runs`'. The values of the different variables and flags are printed on the screen by '`configure`' at the end of the procedure (if no errors occur). **During the configuration, you should pay attention to the information printed by the command '`configure`'.**

A typical output of the `configure` script is shown in Table 7, where the list of the variables that are set during the installation is shown. The user settable variables are: `FC`, `MPIF90`, `MPIEXEC`, `FCFLAGS`, `F77`, `NETCDF`, `NC_INC`, `NC_LIB`, `WGRIB`, `WGRIB2`, `RUNDIR`, `DATADIR` and `SCRIPTDIR`. These variables can be changed by defining them as shell environment variables or by passing their value as a argument in the '`configure`' command line. In case you specify a variable both in the environment and in the command line, the value passed in the command line takes the precedence.

Example (see Table 7): the default Fortran compiler found by `configure` is `FC=gfortran`. You can change the default value in the following ways:

(Bourne shell)

```
$ export FC=ifort
$ export FCFLAGS=-O
$ ./configure
```

or

(C-shell)

```
$ setenv FC ifort
$ setenv FCFLAGS -O
$ ./configure
```

or

(any shell)

```
$ ./configure FC=ifort FCFLAGS=-O
```

All the variables listed before can be configured in a similar way. For example, you can set the run directory (`RUNDIR`) and the data directory (`DATADIR`) to different values:

```
$ ./configure DATADIR=/home/myself/fall3d/mydata RUNDIR=/home/myself/fall3d/myruns
```

Moreover you can specify the installation prefix (root directory for the installation of the binaries) with the flag `--prefix=DIRECTORY` and/or choose to install also the parallel version. Example:

```
$ ./configure --prefix=/home/myself/fall3d --enable-parallel FCFLAGS=-O [...]
```

Table 7: Typical output of the `configure` script

```
[... configure messages ...]
configure: Configuration complete - Fall3d-7.1 (serial)
configure:
configure: Using netCDF 4.2.1
configure: Fortran 90 compiler:        FC=gfortran
configure: Enable parallel version:    --enable-parallel=no
configure: Fortran 90 PAR compiler:    MPIF90=(not used)
configure: Launcher of MPI programs:   MPIEXEC=(not used)
configure: Fortran flags:              FCFLAGS=-O
configure: Fortran 77 compiler:        F77=gfortran
configure: Root directory of netcdf:   NETCDF=/usr/local
configure: Compiler flags for netcdf:  NC_INC=-g -I/usr/local/include
configure: Linker flags for netcdf:    NC_LIB=-L/usr/local/lib -lnetcdff -lnetcdf
configure: Grib files reader           WGRIB=wgrib
configure: Grib2 files reader          WGRIB2=wgrib2
configure: Grib2nc config directory:   GRIBCONFDIR=[...]/Utilities/Grib2nc/config
configure: Install prefix:             --prefix=[...]/fall3d-7.1
configure: Executables install prefix: --exec_prefix=${prefix}
configure: Binary directory:           --bindir=${exec_prefix}/bin
configure: Run directory:              RUNDIR=$HOME/Runs
configure: Data directory:             DATADIR=$HOME/Data
configure: Scripts directory (static): SCRIPTDIR=./Scripts
```

7.5 Selecting the netCDF library

The path of the `netCDF` include files and libraries is defined by the variable `NETCDF`, which specifies the root directory of the `netCDF` installation. In particular, the include files (eg: file `netcdf.inc`) are stored in the directory `$NETCDF/include` and the libraries (eg: file `libnetcdf.a`) are stored in `$NETCDF/lib`. The `configure` script should automatically set the proper value of the `NETCDF` path. This path is searched using a guess algorithm. First of all '`configure`' looks for the program '`nc-config`', provided with the latest versions of `netCDF`; if it is found, `nc-config` is called and the variables `NETCDF`, `NC_INC` and `NC_LIB` are set accordingly. Otherwise, the `NETCDF` path is defined by the location of the program `ncdump`, usually stored in the directory `$NETCDF/bin`. In case '`configure`' is not able to locate your `netCDF` installation, or you want to select another version of `netCDF`, you can manually set the variable `NETCDF`. This cand be done, as for the other variables, either by passing them as an environmental variable, or in the '`configure`' command line:

```
$ ./configure NETCDF=/usr/local/netcdf
```

The variables `NC_INC` and `NC_LIB` represent the flags passed, respectively, to the fortran compiler and to the linker, in order to use `netCDF` (see Table 7 for the typical values). Usually, `NC_INC` and `NC_LIB` are inferred from the value of `NETCDF`.

The variable `GRIBCONFDIR` represents the directory where the configuration files of the utility `Grib2nc` are stored. Just as the other variables, it can be changed by passing a new value to the `./configure` command line or by setting the corresponding environment variable.

7.6 Cleaning directories and uninstalling

After compilation and installation, you can remove the program binaries and object files from the source directory by typing '`make clean`'. To remove the files that '`configure`' has created (so you can compile the package for a different configuration), type '`make distclean`'. This command removes also the Scripts generated by `configure` in the directory `SCRIPTDIR`.

To uninstall FALL3D-7.1 you can type '`make uninstall`' to remove the binary files in the directory `$exec_prefix/bin`. It does not remove the source files and the Scripts.

7.7 Model execution

To run a new simulation named `name` simply create a new directory (or a symbolic link) called `name` in the folder `Runs` and create a new control input file `name.inp` (or simply copy the file Example.inp located in the folder Example, rename it as name.inp and modify it). FALL3D-7.1 and the utility programs are launched using a serie of scripts with some arguments (an option is to create alias for the scripts, so that these can be called directly from any folder). The execution flow is as follows:

1. First, place the meteorological data files in the appropriate folder (or create a symbolic link to data in this folder):

   - `Data/model-grib` for meteo files in grib format or,
   - `Data/model-nc` for meteo files in NetCDF format

   where `model` take one of the following names (see Table 2):

   - `gfs05deg` for GFS forecasts at 0.5^o resolution.
   - `gfs1deg` for GFS forecasts at 1^o resolution.
   - `ncepFNL` for NCEP GFS final analysis (FNL) at 1^o resolution.
   - `ncep1` for CDAS-NCEP/NCAR reanalysis 1 at 2.5^o resolution.
   - `ncep2` for NCEP Reanalysis 2 at 2.5^o resolution.
   - `era40` for ECMWF ERA-40 reanalysis.
   - `eraIn` for ECMWF ERA-Interim reanalysis.
   - `wrf` for WRF-ARW output.
   - `eta` for ETA output.
   - `arpa` for ARPA-SIM output.
   - `calmet62` for CALMET (version 6.2) output.
   - `profile` for vertical profile.

   NOTE: The scripts assume that files in folder `Data/model-grib` are named `name.model.grib` and files in folder `Data/model-nc` are named `name.model.nc` (*e.g.* `name.wrf.nc` for WRF-ARW output files located in folder `Data/wrf-nc`, `name.eraIn.grib` for ERA-Interim grib files located in folder `Data/eraIn-grib`, etc).

2. If necessary (only for meteo files in grib format), run `wgrib/wgrib2` and `GRIB2NC`. For this, you have to launch one of the following scripts:

   - `Script-gfs05deg-to-nc name`
     where `name` is the name of the current run. This decodes the file `name.gfs05deg.grib` (GFS forecasts at 0.5^o resolution), placed in the folder `Data/gfs05deg-grib`, and creates the file `name.gfs05deg.nc` in the folder `Data/gfs05deg-nc` for subsequent execution of `SETDBS`.
   - `Script-gfs1deg-to-nc name`
     where `name` is the name of the current run. This decodes the file `name.gfs1deg.grib` (GFS forecasts at 1^o resolution), placed in the folder `Data/gfs1deg-grib`, and creates the file `name.gfs1deg.nc` in the folder `Data/gfs1deg-nc` for subsequent execution of `SETDBS`.
   - `Script-ncepFNL-to-nc name`
     where `name` is the name of the current run. This decodes the file `name.ncepFNL.grib` (final analysis at 1^o resolution), placed in the folder `Data/ncepFNL-grib`, and creates the file `name.ncepFNL.nc` in the folder `Data/ncepFNL-nc` for subsequent execution of `SETDBS`.

- `Script-ncep1-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.ncep1.grib` (reanalysis 1), placed in the folder `Data/ncep1-grib`, and creates the file `name.ncep1.nc` in the folder `Data/ncep1-nc` for subsequent execution of `SETDBS`.
  NOTE: This script can be used for `ncep1` files already downloaded in grib-format. Currently `ncep1` files are available only in nc-format and in this case `Script-ncep1-cat-nc name` should be used.
- `Script-ncep2-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.ncep2.grib` (reanalysis 2), placed in the folder `Data/ncep2-grib`, and creates the file `name.ncep2.nc` in the folder `Data/ncep2-nc` for subsequent execution of `SETDBS`.
  NOTE1: This script can be used for `ncep2` files already downloaded in grib-format. Currently `ncep2` files are available only in nc-format and in this case `Script-ncep2-cat-nc name` should be used.
  NOTE2: Variable files must be named with standard NCEP names, i.e. `hgt.nc, rhum.nc, omega.grib, uwnd.nc, vwnd.nc, etc`.
- `Script-ncep1-cat-nc name`
  where `name` is the name of the current run. This merges the files `variable1.nc`, `variable2.nc`, etc. (reanalysis 1), placed in the folder `Data/ncep1-nc`, and creates the file `name.ncep1.nc` in the folder `Data/ncep1-nc` for subsequent execution of `SETDBS`.
- `Script-ncep2-cat-nc name`
  where `name` is the name of the current run. This merges the files `variable1.nc`, `variable2.nc`, etc. (reanalysis 2), placed in the folder `Data/ncep2-nc`, and creates the file `name.ncep2.nc` in the folder `Data/ncep2-nc` for subsequent execution of `SETDBS`.
- `Script-era40-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.era40.grib` (ECMWF ERA-40), placed in the folder `Data/era40-grib`, and creates the file `name.era40.nc` in the folder `Data/era40-nc` for subsequent execution of `SETDBS`.
- `Script-eraIn-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.eraIn.grib` (ECMWF ERA-Interim), placed in the folder `Data/eraIn-grib`, and creates the file `name.eraIn.nc` in the folder `Data/eraIn-nc` for subsequent execution of `SETDBS`.
- `Script-eta-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.eta.grib` (ETA model output), placed in the folder `Data/eta-grib`, and creates the file `name.eta.nc` in the folder `Data/eta-nc` for subsequent execution of `SETDBS`.
- `Script-arpa-to-nc name`
  where `name` is the name of the current run. This decodes the file `name.arpa.grib` (ARPA-SIM model output), placed in the folder `Data/arpa-grib`, and creates the file `name.arpa.nc` in the folder `Data/arpa-nc` for subsequent execution of `SETDBS`.
  NOTE: If an alias for the scripts has not been previously set, the user must run `wgrib/wgrib2` and `GRIB2NC` from the `Scripts` folder and provide the full path for the grib file.
  NOTE2: For some of the scripts it may be necessary to modify some variables depending on the specific problem.

3. Run the `SETDBS` utility program to generate the file `name.dbs.nc` in the folder `Runs/name`:

   - `Script-SetDbs name model`

   where `name` is the name of the current run and `model` is one of the following options:

   - `gfs05deg/gfs1deg (for global model forecasts)`
   - `ncepFNL/ncep1/ncep2/era40/eraIn (for reanalyses)`

- `wrf/eta/arpa (for mesoscale models)`
- `profile/calmet62 (for other options)`

4. Run the `SETTGSD` utility program to generate the file `name.tgsd` in the folder `Runs/name`:

   - `Script-SetTgsd name`

   where `name` is the name of the current run. Alternatively, the TGSD file can be created by the user directly.

5. Run the `SETSRC` utility program to generate the files `name.src` and `name.grn` in the folder `Runs/name`:

   - `Script-SetSrc name`

   where `name` is the name of the current run.

6. Run `FALL3D-7.1` in either serial or parallel versions:

   - `Script-Fall3d_ser name`

   to run `FALL3D-7.1` serial, where `name` is the name of the current run;

   - `Script-Fall3d_par name ncpu ngroup`

   to run `FALL3D-7.1` parallel. Note that, in general, this script has to be edited and modifyed depending on each particular queuing system.

7. Run the `FALL3D2GMT` utility program to postprocess results:

   - `Script-Fall3d2GMT name`

   where `name` is the name of the current run. Note that this makes use of GMT and the convert utilities (from ImageMagic), not included in the distribution.

Appendices

Appendix A. Governing equations and parameterizations

In FALL3D-7.1 it is assumed that the main factors controlling atmospheric transport of ash are wind advection, turbulent diffusion, and gravitational settling of particles. This assumption does not hold in the proximal region that can be extended for large eruptions (having high eruption columns and large mass eruption rates), where eruption clouds can spread at the NBL as a gravity current. A simple analytical model describing this effect can be used in FALL3D-7.1.
Neglecting particle-particle interaction effects (collisions, aggregation, *etc.*), the Eulerian form of the continuity equation written in a generalized coordinate system (X, Y, Z) is (Byun and Schere, 2006; Costa et al., 2006):

$$\begin{aligned}&\frac{\partial C}{\partial t} + V_X\frac{\partial C}{\partial X} + V_Y\frac{\partial C}{\partial Y} + (V_Z - V_{sj})\frac{\partial C}{\partial Z} = -C\nabla\cdot\mathbf{V} + C\frac{\partial V_{sj}}{\partial Z}\\ &+\frac{\partial}{\partial X}\left(\rho_* K_X\frac{\partial C/\rho_*}{\partial X}\right) + \frac{\partial}{\partial Y}\left(\rho_* K_Y\frac{\partial C/\rho_*}{\partial Y}\right) + \frac{\partial}{\partial Z}\left(\rho_* K_Z\frac{\partial C/\rho_*}{\partial Z}\right) + S_*\end{aligned} \tag{1}$$

where C is the transformed concentration, $\mathbf{V} = (V_X, V_Y, V_Z)$ is the transformed wind speed, K_X, K_Y and K_Z are the diagonal terms of the transformed eddy diffusivity tensor, ρ_* is the transformed atmospheric density, and S_* is the transformed source term. FALL3D-7.1 solves Eq. (1) for each particle class j using a curvilinear terrain-following coordinate system ($X = mx$, $Y = my$, $z \to Z$), where m is the map scale factor and $Z = z - h(x, y)$, with $h(x, y)$ denoting the topographic elevation, and (x, y, z) are the Cartesian coordinates. The scaling factors for this particular transformation are given in Table 8 (Byun and Schere, 2006). The generic particle class j is defined by a triplet of values characterizing each particle (d_p, ρ_p, F_p), that are, respectively, diameter, density, and a shape factor. For d_p we use the equivalent diameter d, which is the diameter of a sphere of equivalent volume. For the shape factor F_p we choose the sphericity ψ, which is the ratio of the surface area of a sphere with diameter d to the surface area of the particle. In our approximation, each triplet (d, ρ_p, ψ) is sufficient to define the settling velocity. Effect of Earth's curvature are considered when the lat-lon coordinate system is used through the Jacobian of the transformation.

Parameter	Scaling
Coordinates	$X = mx; \quad Y = my; \quad Z = z - h(x, y)$
Horizontal Velocities	$V_X = mv_x; \quad V_Y = mv_y$
Vertical velocity	$(V_Z - V_{Sj}) = J^{-1}\left[(v_z - v_{sj}) - m\left(v_x\frac{\partial h}{\partial x} + v_y\frac{\partial h}{\partial y}\right)\right]$
Diffusion Coefficients	$K_X = K_x; \quad K_Y = K_y; \quad K_Z \simeq K_z J^{-2}$
Concentration	$C = cJ/m^2$
Density	$\rho_* = \rho J/m^2$
Source Term	$S_* = SJ/m^2$

Table 8: Scaling factors for a terrain-following coordinate system ($x = mX$, $y = mY,$, $z \to Z$). (x, y, z) are the Cartesian coordinates, m the map scale factor (for the UTM coordinate system $m = 1$) and J is the determinant of the Jacobian of the coordinate system transformation.

Eddy Diffusivity Tensor

In FALL3D-7.1 only the diagonal components of the Eddy Diffusivity Tensor, *i.e.* the vertical K_z and the horizontal $K_h = K_x = K_y$ components, are considered.
The available choices for describing the vertical component K_z are:

1. Option CONSTANT, *i.e.* $K_z = constant$, where the constant value is assigned by the user;

2. Option `SIMILARITY`. In this case, inside the Atmospheric Boundary Layer (ABL), `FALL3D-7.1` evaluates K_z as:

$$K_z = \begin{cases} \kappa u_* z \left(1 - \frac{z}{h}\right) \left(1 + 9.2 \frac{h}{L} \frac{z}{h}\right)^{-1} & h/L \geq 0 \quad \text{stable} \\ \kappa u_* z \left(1 - \frac{z}{h}\right) \left(1 - 13 \frac{h}{L} \frac{z}{h}\right)^{1/2} & h/L \leq 0 \quad \text{unstable} \end{cases} \tag{2}$$

where κ is the von Karman constant ($\kappa = 0.4$), u_* is the wind friction velocity, h is the ABL height, and L is the Monin-Obukhov length (see Costa et al., 2006). The expression above comes from an extension of the Monin-Obukhov similarity theory to the entire ABL (Ulke, 2000). On the other hand, above the ABL ($z/h > 1$), K_z is considered as a function of the local vertical wind gradient, a characteristic length scale l_c, and a stability function F_c which depends on the Richardson number Ri:

$$K_z = l_c^2 \left| \frac{\partial U}{\partial z} \right| F_c(Ri) \tag{3}$$

where $U = \sqrt{y_x^2 + u_y^2}$. For l_c and F_c, `FALL3D-7.1` adopts the relationship used by the CAM-3.0 model (Collins et al., 2004):

$$l_c = \left(\frac{1}{\kappa z} + \frac{1}{\lambda_c} \right)^{-1} \tag{4}$$

$$F_c(Ri) = \begin{cases} \dfrac{1}{1 + 10Ri(1 + 8Ri)} & \text{stable} \quad (Ri > 0) \\ \sqrt{1 - 18Ri} & \text{unstable} \quad (Ri < 0) \end{cases} \tag{5}$$

where λ_c is the so-called asymptotic length scale ($\lambda_c \approx 30$m).

The available choices for describing the horizontal component $K_h = K_x = K_y$ are:

1. Option `CONSTANT`, *i.e.* $K_h = constant$, where the constant value is assigned by the user;

2. Option `RAMS`. In this case, a large eddy parameterization as the one used by the RAMS model (Pielke et al., 1992) can be used for evaluating K_h:

$$K_h = Pr_t \max \left(k_m; (C_S \Delta)^2 \sqrt{\left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right)^2 + 2 \left[\left(\frac{\partial v_x}{\partial x} \right)^2 + \left(\frac{\partial v_y}{\partial y} \right)^2 \right]} \right) \tag{6}$$

where Pr_t is the turbulent Prandtl number (typically $Pr_t \approx 1$), $k_m = 0.075\Delta^{4/3}$, $\Delta = \sqrt{\Delta x \Delta y}$, Δx and Δy are the horizontal grid spacings, and C_S is a constant ranging from 0.135 to 0.32.

3. Option `CMAQ`. In this case, the horizontal diffusion is evaluated as in the CMAQ model (Byun and Schere, 2006):

$$\frac{1}{K_h} = \frac{1}{K_{ht}} + \frac{1}{K_{hn}} \tag{7}$$

where:

$$K_{ht} = \alpha^2 \Delta x \Delta y \sqrt{\left(\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} \right)^2 + \left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y} \right)^2} \tag{8}$$

$$K_{hn} = K_{hf} \left(\frac{\Delta x_f \Delta y_f}{\Delta x \Delta y} \right) \tag{9}$$

where the numeric constant $\alpha = 0.28$ and the values of K_{hf} and $\Delta x_f = \Delta y_f$ depend on the algorithm. Using this parameterization, for a large grid size the effect of the transportive dispersion is minimized, whereas for a small grid size the numerical diffusion term is reduced (Byun and Schere, 2006). Thanks to the heuristic relationship (7), the smaller of K_{ht} and K_{hn} dominates. In our case we set $K_{hf} = 8000$ m^{2}s^{-1} for $\Delta x_f = \Delta y_f = 4$ km and a minimum value for K_h equal to $k_m = 0.075\Delta^{4/3}$ was imposed.

Settling velocity models

There are several semi-empirical parameterizations for the particle settling velocity v_s if one assumes that particles settle down at their terminal velocity:

$$v_s = \sqrt{\frac{4g\,(\rho_p - \rho_a)\,d}{3C_d\rho_a}} \tag{10}$$

where ρ_a and ρ_p denote air and particle density, respectively, d is the particle equivalent diameter, g is the gravity acceleration, and C_d is the drag coefficient. C_d depends on the Reynolds number, $Re = dv_s/\nu_a$ ($\nu_a = \mu_a/\rho_a$ is the kinematic viscosity of air, and μ_a the dynamic viscosity). In FALL3D-7.1 different options are possible for estimating settling velocity, such as:

1. ARASTOOPOUR model (Arastoopour et al., 1982):

$$C_d = \begin{cases} \dfrac{24}{Re}(1 + 0.15Re^{0.687}) & Re \leq 988.947 \\ 0.44 & Re > 988.947 \end{cases} \tag{11}$$

   valid for spherical particles only.

2. GANSER model (Ganser, 1993):

$$C_d = \frac{24}{ReK_1}\left\{1 + 0.1118\,(Re\,K_1K_2)^{0.6567}\right\} + \frac{0.4305K_2}{1 + \dfrac{3305}{Re\,K_1K_2}} \tag{12}$$

   where $K_1 = 3/[(d_n/d) + 2\psi^{-0.5}]$, $K_2 = 10^{1.8148(-\mathrm{Log}\psi)^{0.5743}}$ are two shape factors (d_n is the average between the minimum and the maximum axis, d is the equal volume sphere), and ψ is the particle sphericity ($\psi = 1$ for spheres). For calculating the sphericity is practical to use the concepts of "operational" and "working sphericity", ψ_{work} introduced by Wadell (1933); Aschenbrenner (1956), which are based on the determination of the volume and of the three dimensions of a particle respectively:

$$\psi_{work} = 12.8\frac{(P^2Q)^{1/3}}{1 + P(1+Q) + 6\sqrt{1 + P^2(1+Q^2)}} \tag{13}$$

   with $P = S/I$, $Q = I/L$, where L is the longest particle dimension, I is the longest dimension perpendicular to L, and S is the dimension perpendicular to both L and I.

3. WILSON model (Walker et al., 1971; Wilson and Huang, 1979) using the interpolation suggested by Pfeiffer et al. (2005):

$$C_d = \begin{cases} \dfrac{24}{Re}\varphi^{-0.828} + 2\sqrt{1-\varphi} & Re \leq 10^2 \\ 1 - \dfrac{1 - C_d|_{Re=10^2}}{900}(10^3 - Re) & 10^2 \leq Re \leq 10^3 \\ 1 & Re \geq 10^3 \end{cases} \tag{14}$$

   where $\varphi = (b + c)/2a$ is the particle aspect ratio ($a \geq b \geq c$ denote the particle semi-axes).

4. DELLINO model (Dellino et al., 2005):

$$v_s = 1.2605\frac{\nu_a}{d}\left(Ar\,\xi^{1.6}\right)^{0.5206} \tag{15}$$

   where $Ar = gd^3(\rho_p - \rho_a)\rho_a/\mu_a^2$ is the Archimedes number, g the gravity acceleration, and ξ is a particle shape factor (sphericity to circularity ratio). It is recommended to not extrapolate this option for particle diameters beyond the range used in the experiments by Dellino et al. (2005).

Since for FALL3D-7.1 the primary particle shape factor is the sphericity ψ, for sake of simplicity, φ in (14) and ξ in (15) are calculated by approximating particles as prolate ellipsoids (the same approximation is used for estimating d_n).

Particle aggregation

For computational reasons ash particle aggregation is assumed to occur within the eruption plume affecting the original TGSD which is modified considering an effective aggregate class and depleting particle classes finer than the aggregate class itself. A few possibilities are available in FALL3D-7.1 such as

1. NONE option that neglect aggregation;
2. PERCENTAGE option that simply subtracts a constant percentage of ash from each particle class having diameter smaller than the user-defined aggregate diameter with a user-defined aggregate density (e.g. Sulpizio et al., 2012);
3. CORNELL option that is similar to the parameterization proposed by Cornell et al. (1983) as used in Costa et al. (2012);
4. COSTA option based on Costa et al. (2010) model. For computational reasons all the three options assume that ash aggregation occurs mainly within the eruption column and affect the original TGSD (described by filename.tgsd) by creating an effective particle distribution (described by filename.grn). Option COSTA can be used only with source model PLUME.

Source term

FALL3D-7.1 reads the time-dependent source term (mass released per unit time at each grid point) from an external file. This file can be generated by the SETSRC utility program, choosing among different options such as:

1. POINT_SOURCE that emits mass from a point source only;
2. SUZUKI that describe the eruptive column as a mushroom-like shape Suzuki (1983); Pfeiffer et al. (2005)
3. PLUME that uses an eruptive column model based on the Buoyant Plume Theory (based on Bursik, 2001; Folch et al., 2012).
4. RESUSPENSION that describes resuspension of ash deposited on the ground remobilized by wind. This option is described more in detail below.

Resuspension of ash

Saltation impact represents the most effective mechanism for resuspension of smaller-size particles in soils (Shao et al., 1993). When the intensity of wind blowing across a granular soil exceeds a certain threshold, grain particles begin to saltate. Experiments with sand-sized particles show that the impact of saltating mid-size grains (larger than about $50\,\mu m$) breaks the cohesive forces of smaller particles, enhancing their suspension when falling back to ground. For this reason, the emission rate (vertical flux of particles), defined as the mass emitted per unit of area and time, strongly depends on the horizontal (saltation) flux of larger particles. FALL3D-7.1 uses different emission schemes for ash resuspension by wind (see Folch et al., 2014):

1. Emission scheme 1 (Westphal et al., 1987) computes the emission rate as:

$$F_V = \begin{cases} 0 & u_* < u_{*t} \\ 10^{-5} u_*^4 & u_* \geq u_{*t} \end{cases} \tag{16}$$

where F_V is the vertical flux (in kg $\mathrm{m}^{-2}\mathrm{s}^{-1}$), occurring only above a (constant) threshold friction velocity u_{*t}. An important limitation of (16) is that the vertical flux does not depend on particle size or soil moisture. Although very simple, this parameterization can be useful when information on soil characteristics (*e.g.* particle sizes and densities, moisture, roughness, etc.) is not available or poorly constrained.

2. Emission scheme 2 (Marticorena and Bergametti, 1995; Marticorena et al., 1997) computes the emission rate as:

$$F_V(d) = \begin{cases} 0 & u_* < u_{*t}(d) \\ \dfrac{K\rho_a u_*}{g}\left(u_*^2 - u_{*t}^2(d)\right) & u_* \geq u_{*t}(d) \end{cases} \tag{17}$$

where K is a soil texture coefficient equal to $K = 5.4 \times 10^{-4}$ m^{-1} from experiments, u_* denotes the wind friction velocity, and u_{*t} is the threshold friction velocity given by:

$$u_{*t} = \begin{cases} \frac{0.129K}{(1.928Re^{0.092}-1)^{0.5}} & 0.03 < Re \leq 10 \\ 0.129K(1 - 0.0858e^{-0.0617(Re-10)}) & Re > 10 \end{cases} \tag{18}$$

with $K = \sqrt{\frac{\rho_p g d}{\rho_a}\left(1 + \frac{0.006}{\rho_p g d^{2.5}}\right)}$ and $Re = 1331 \times d^{1.56}$ (the lower bound of the fit corresponds to particles of $\approx 10\,\mu m$ in size). Please note that inn the relationship above, ρ_p and ρ_a are particle and air densities (expressed in g/cm^3), g is gravity (in cm/s^2), d is the particle size (in cm), Re is the Reynolds number parameterized as a function of the particle size, and u_{*t} is given in cm/s.

3. Emission scheme 3 (Shao et al., 1993; Shao and Leslie, 1997; Shao and Lu, 2000) computes the emission rate as:

$$F_V(d, d_s) = \frac{\alpha(d, d_s)}{u_{*t}^2(d)} F_H(d_s) \tag{19}$$

where α (units of m s^{-2}) is a coefficient of blasting efficiency determined experimentally (Shao and Leslie, 1997) and F_H is the horizontal flux (units of kg m^{-1} s^{-1}) of saltating particles of size d_s:

$$F_H(d_s) = \begin{cases} 0 & u_* < u_{*t}(d_s) \\ c_o \frac{\rho_a u_*^3}{g}\left(1 - \frac{u_{*t}^2(d_s)}{u_*^2}\right) & u_* \geq u_{*t}(d_s) \end{cases} \tag{20}$$

and c_o is an empirical dimensionless constant close to 1. The threshold friction velocity $u_{*t}(d)$ is given by:

$$u_{*ts} = \sqrt{0.0123\left(\frac{\rho_p g d}{\rho_a} + \frac{\gamma}{\rho_a d}\right)} \tag{21}$$

where γ is a parameter ranging between 1.65×10^{-4} and 5×10^{-4} kg/s^2 (a value of 3×10^{-4} kg/s^2 is assumed in FALL3D-7.1).

NOTE: in the current version, simulation of resuspension is possible only in combination with WRF-ARW meteorological data.

Spreading of the volcanic cloud at the NBL

When the option GRAVITY_CURRENT is used an analytical model describing the spreading of the volcanic cloud at NBL as a gravity current (e.g., Woods and Kienle, 1994; Sparks et al., 1997) is coupled to the ADS transport (see Costa et al., 2013). In summary this option consists of adding an effective radial velocity field to the wind field. The radial wind field due to the gravitational spreading of the current is centered above the vent in the umbrella region and extended up to a radius R in accordance with:

$$\begin{cases} u_b(R) = \left(\dfrac{2\lambda N q}{3\pi}\right)^{1/2} \dfrac{1}{\sqrt{R}} & \text{for } R \leq R_p \text{ and } H_U - \frac{h}{2} \leq z \leq H_U + \frac{h}{2} \\ u_b(R) = 0 & \text{for } R > R_p \text{ or } z < H_U - \frac{h}{2} \text{ or } z > H_U + \frac{h}{2} \end{cases} \tag{22}$$

where λ is an empirical constant, and N is the frequency of Brunt–Vaisala due to the ambient stratification, q is the volumetric flow rate into the umbrella region, H_U denotes the level (NBL), and h the thickness of umbrella region that is assumed to scale with u_b as $h = u_b/(\lambda N)$. Within this region variation of the velocity field with the radial distance r is calculated as:

$$u_b(r) = \frac{3}{4} u_b(R) \frac{R}{r}\left(1 + \frac{1}{3}\frac{r^2}{R^2}\right) \tag{23}$$

The radial field is considered negligible at distances larger than a critical radius R_p (Costa et al., 2013).

Wet deposition

As a first approach, wet deposition is assumed below the Planetary Boundary Layer (PBL) only. Using this approximation only the total rate is necessary to describe wet deposition that is parameterized as (e.g., Jung and Shao, 2006):

$$\frac{dC}{dt} = -L\,C = -A\,P^B\,C \tag{24}$$

where P is the precipitation rate in mm h^{-1}, A and B are two empirical constants ($A = 8.4 \cdot 10^{-5}$ and $B = 0.79$ respectively). Two critical cut-off size at 1 and 100 μms are assumed.

Appendix B. Example of control input file

This is an example (not from a real case) of control input file. Comments begin with an exclamation symbol.

```
!
!  ------------------------------------------
!
!  EXAMPLE OF FALL3D INPUT FILE
! VERSION: 7.1
!
!  ------------------------------------------
!
!  ------------------------------------------
!  Blocks read by Fall3d and utility programs
!  ------------------------------------------
!
TIME_UTC
YEAR = 2008
MONTH = 04
DAY = 29
BEGIN_METEO_DATA_(HOURS_AFTER_00) = 0
TIME_STEP_METEO_DATA_(MIN) = 60
END_METEO_DATA_(HOURS_AFTER_00) = 24
ERUPTION_START_(HOURS_AFTER_00) = 0 3.5
ERUPTION_END_(HOURS_AFTER_00) = 7
RUN_END_(HOURS_AFTER_00) = 10
RESTART = NO
!
GRID
COORDINATES = LON-LAT
LON_LAT
LONMIN = 14.0
LONMAX = 16.0
LATMIN = 36.5
LATMAX = 38.5
LON_VENT = 15.0
LAT_VENT = 37.5
VENT_HEIGHT_(M) = 3000.
NX = 51
NY = 51
ZLAYER_(M) FROM 0.  TO 8000.  INCREMENT 500.
!
!  ------------------------------------------
!  Block read by SetTGsd utility program
!  ------------------------------------------
!
GRANULOMETRY
DISTRIBUTION = GAUSSIAN
NUMBER_OF_CLASSES = 6
FI_MEAN = 2.5
FI_DISP = 1.5
FI_RANGE = 2.  7.
```

```
DENSITY_RANGE = 1200 2300
SPHERICITY_RANGE = 0.9 0.9
MIXING_FACTOR = 0.5
!
!  ------------------------------------------
!  Blocks read by SetSrc utility program
!  ------------------------------------------
!
SOURCE
!
!  SOURCE_TYPE options:  POINT/SUZUKI/PLUME/RESUSPENSION
!
SOURCE_TYPE = plume
!
POINT_SOURCE
!
HEIGHT_ABOVE_VENT_(M) = 3000.  6000.
MASS_FLOW_RATE_(KGS) = ESTIMATE-WOODHOUSE
!
SUZUKI_SOURCE
!
HEIGHT_ABOVE_VENT_(M) = 3000.  6000.
MASS_FLOW_RATE_(KGS) = ESTIMATE-WOODHOUSE
A = 4.
L = 1.
!  PLUME_SOURCE
!
SOLVE_PLUME_FOR = MFR
MFR_SEARCH_RANGE = 3.0 7.0
HEIGHT_ABOVE_VENT_(M) = 6000.
MASS_FLOW_RATE_(KGS) = 1d3 1d4
EXIT_VELOCIY_(MS) = 200.
EXIT_TEMPERATURE_(K) = 1073.
EXIT_WATER_FRACTION_(%) = 1.
!
RESUSPENSION_SOURCE
!
MAX_RESUSPENSION_SIZE_(MIC) = 100
DEPOSIT_THRESHOLD_(KGM2) = 1
MAX_INJECTION_HEIGHT_(M) = 1000
EMISSION_SCHEME = WESTPHAL
EMISSION_FACTOR = 1.0
THRESHOLD_UST = 0.3
MOISTURE_CORRECTION = no
!
AGGREGATION
!
AGGREGATION_MODEL = Cornell
FI_AGGREGATES = 2.
DENSITY_AGGREGATES = 350.
VSET_FACTOR = 1.0
PERCENTAGE_(%) = 20.
FRACTAL_EXPONENT = 2.99
!
```

```
AEROSOLS
!
SO2 = no
SO2_PERCENTAGE_(%) = 1.
!
GRAVITY_CURRENT
!
GRAVITY_CURRENT = no
C_FLOW_RATE = 1d4
LAMBDA_GRAV = 0.2
K_ENTRAIN = 0.1
BRUNT_VAISALA = 0.02
!
!  ------------------------------------------
!  Block read by Fall3d
!  ------------------------------------------
!
FALL3D
!
TERMINAL_VELOCITY_MODEL = ganser
VERTICAL_TURBULENCE_MODEL = CONSTANT
VERTICAL_DIFFUSION_COEFFICIENT_(M2/S) = 500.
HORIZONTAL_TURBULENCE_MODEL = CONSTANT
RAMS_CS = 0.3
HORIZONTAL_DIFFUSION_COEFFICIENT_(M2/S) = 5000.
WET_DEPOSITION = yes
!
OUTPUT
!
POSTPROCESS_TIME_INTERVAL_(HOURS) = 1.
POSTPROCESS_3D_VARIABLES = YES
POSTPROCESS_CLASSES = YES
TRACK_POINTS = YES
!
!  ------------------------------------------
!  Blocks read by Postprocess utility program(s)
!  ------------------------------------------
!
POSTPROCESS
!
CROP_DOMAIN
LONMIN = 14.0
LONMAX = 16.0
LATMIN = 36.5
LATMAX = 38.5
!
!  Meteo
!
MAP_TEMPERATURE = yes
MAP_VELOCITY = yes
Z_CUTS_(M) = 1000 5000
!
!  Time independent variables
!
```

```
MAP_TOPOGRAPHY = no
UNITS = M
CONTOUR_LEVELS = 1.  100.  500.  1000.  1500.  2000.  2500.
!
!  Deposit variables
!
MAP_TOTAL_LOAD = no
UNITS = KG/M2
CONTOUR_LEVELS = 0.1 0.5 1.  5.  10.  50.
!
MAP_WET_LOAD = no
UNITS = KG/M2
CONTOUR_LEVELS = 0.1 0.5 1.  5.
!
MAP_CLASS_LOAD = no
UNITS = KG/M2
CONTOUR_LEVELS = 0.1 0.5 1.  5.  10.  50.
!
MAP_CLASS_WET = yes
UNITS = KG/M2
CONTOUR_LEVELS = 0.1 0.5 1.  5.
!
MAP_DEPOSIT_THICKNESS = no
DEPOSIT_DENSITY_(KG/M3) = 1100.0 (Default value 1000.)
UNITS = MM (Possibilities:  MM/CM/M)
CONTOUR_LEVELS = 0.1 0.5 1.  5.  10.
!
!  Ground level variables
!
MAP_CONCE_GROUND = no
UNITS = G/M3
CONTOUR_LEVELS = 0.001 0.01 0.1 1.
!
MAP_PMxx_GROUND = no
UNITS = G/M3
CONTOUR_LEVELS = 1d-5 1d-4 1d-3
!
!  Airborne variables
!
MAP_COLUMN_MASS = no
UNITS = G/M2
CONTOUR_LEVELS = 1.  10.  100.
!
MAP_COLUMN_PMxx = no
UNITS = G/M2
CONTOUR_LEVELS = 0.1 1.  10.  100.
!
MAP_FLIGHT_LEVEL = no
UNITS = G/M3
CONTOUR_LEVELS = 0.001 0.01 0.1
!
MAP_AOD = no
UNITS = NONE
CONTOUR_LEVELS = 0.1 0.25 0.5 0.75 1 2
```

Appendix C. The NetCDF format

NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data (http://www.unidata.ucar.edu/software/netcdf/).
FALL3D-7.1 uses the standard NetCDF format for both database input file (`name.dbs.nc`) and results output file (`name.res.nc`). There is a good number of open-source codes to view, analyze or manipulate NetCDF files, for example:

- ncview and ncdump (http://opendap.org/download/nc_clients.html).
- Panoply (http://www.giss.nasa.gov/tools/panoply/).
- GMT (http://gmt.soest.hawaii.edu/)
- GrADS (http://www.iges.org/grads/).
- NCL, the NCAR Command Language (http://www.ncl.ucar.edu/).
- GRASS (http://grass.osgeo.org/)
- QGIS (http://www.qgis.org)
- R (http://www.r-project.org/)

pcoord
pdate
itime1 itime2
nz
z(1) ux(1) uy(1) T(1)
...
z(nz) ux(nz) uy(nz) T(nz)
itime3 itime4
...

Table 9: Format of the meteo data file `name.profile.dat` for the `PROFILE` case. Repeat this block for each meteo time increment.

Appendix D. Format of the meteo profile file (`name.profile`)

For the profile option, the utility `SetDbs` needs an ASCII file containing the definition of the vertical wind and temperature profile and a topography file of the domain in GRD format. In this case wind velocities are assumed constant on all the domain in a terrain-following coordinate system. The remaining variables are assumed with the values of the Standard Atmosphere. The format of the profile file (`name.profile`) is described in Table 9 and the meaning of the used symbols is the following:

- `pcoord`: Coordinates where the profile was measured; either as UTM or lon-lat coordinates.
- `pdate`: Starting time when the profile was measured; the format of the date is `yyyymmdd`, *i.e.* year, month, day.
- `itime1`: Initial time in sec after the starting time `pdate` of validity of the meteo data contained in the following `nz` layers.
- `itime2`: Final time in sec after the starting time `pdate` of validity of the meteo data contained in the following `nz` layers.
- `nz`: Number of the database vertical layers.
- `z`: Vertical coordinate of the layer (in m a.s.l.).
- `ux`: wind x-velocity (in m/s).
- `uy`: wind y-velocity (in m/s).
- `T`: temperature T-velocity (in ^{o}C).

Appendix E. The GRD format

The structure of a GRD format file is described in Table 10 and the meaning of the used symbols is the following:

- `NX` : Number of grid points along x-direction.
- `NY` : Number of grid points along y-direction.
- `XO` : x-coordinate (UTM in m) of the grid bottom left corner point.
- `XF` : x-coordinate (UTM in m) of the grid top right corner point.
- `YO` : y-coordinate (UTM in m) of the grid bottom left corner point.
- `YF` : y-coordinate (UTM in m) of the grid top right corner point.
- `VAL` : Value at each grid point. It consists of an array of `NX`×`NY` values stored starting from the bottom-left corner and moving towards right then up towards the top-right corner.

NX	NY		
XO	XF		
YO	YF		
MAX(v)	MIN(v)		
VAL(i,1)	...	...	i=1:NX
...	...	...	
VAL(i,j)	...	...	i=1:NX
...	...	...	
VAL(i,NY)	...	...	i=1:NX

Table 10: Format of a GRD file `name.grd`.

Appendix F. Further reading

The following is a list of publications related to FALL3D:

1. Costa, A., Macedonio, G., Folch, A. (2006). A three-dimensional Eulerian model for transport and deposition of volcanic ashes. Earth Planet. Sci. Lett., 241 (3-4), 634-647, doi: 10.1016/j.epsl.2005.11.019.

2. Folch, A., Jorba, O., and Viramonte, J. (2008). Volcanic ash forecast - application to the May 2008 Chaitén eruption, Nat. Hazards Earth Syst. Sci., 8, 927-940.

3. Scollo, S., A. Folch, A. Costa (2008). A parametric and comparative study of different tephra fallout models, J. Volcanol. Geotherm. Res., 176, 199-211, doi: 10.1016/j.jvolgeores.2008.04.002.

4. Folch A., C. Cavazzoni, A. Costa, G. Macedonio (2008). An automatic procedure to forecast tephra fallout, J. Volcanol. Geotherm. Res., 177, 767-777, doi: 10.1016/j.jvolgeores.2008.01.046 .

5. Macedonio G., A. Costa, A. Folch (2008). Ash fallout scenarios at Vesuvius: Numerical simulations and implications for hazard assessment, J. Volcanol. Geotherm. Res., 178, 366-377, doi: 10.1016/j.jvolgeores.2008.08.014.

6. Folch A., Costa A., Macedonio G. (2009). FALL3D: A Computational Model for Volcanic Ash Transport and Deposition, Comput. Geosci., 35, 1334-1342, doi: 10.1016/j.cageo.2008.08.008.

7. Scollo S., Prestifilippo M., Spata G., D'Agostino M., Coltelli M. (2009). Monitoring and forecasting Etna volcanic plumes, Nat. Hazards Earth Syst. Sci., 9, 1573-1585.

8. Costa A., A. Folch, G. Macedonio (2010). A Model for Wet Aggregation of Ash Particles in Volcanic Plumes and Clouds: I. Theoretical Formulation, J. Geophys. Res., 115, B09201, doi:10.1029/2009JB007175.

9. Folch A., A. Costa, A. Durant,G. Macedonio (2010). A Model for Wet Aggregation of Ash Particles in Volcanic Plumes and Clouds: II. Model Application, J. Geophys. Res., 115, B09202, doi:10.1029/2009JB007176.

10. Folch A., Sulpizio R. (2010). Evaluating long-range volcanic ash hazard using supercomputing facilities: application to Somma-Vesuvius (Italy), and consequences for civil aviation over the Central Mediterranean Area, Bull. Volc., 72 (9), 1039-1059, doi:10.1007/s00445-010-0386-3.

11. Scollo S., A. Folch, M. Coltelli, V.J. Realmuto (2010). Three-dimensional volcanic aerosol dispersal: A comparison between Multiangle Imaging Spectroradiometer (MISR) data and numerical simulations, J. Geophys. Res., 115, D24210, doi:10.1029/2009JD013162.

12. Corradini S., Merucci L., Folch A. (2011). Volcanic Ash Cloud Properties: Comparison Between MODIS Satellite Retrievals and FALL3D Transport Model, IEEE Geoscience and Remote Sensing Letters, 8, 248-252, doi:10.1109/LGRS.2010.2064156.

13. Folch A., Costa A., Basart S. (2012). Validation of the FALL3D ash dispersion model using observations of the 2010 Eyjafjallajokull volcanic ash cloud, Atmos. Environ., 48, 165-183, doi:10.1016/j.atmosenv.2011.06.072.

14. Scaini C., Folch A., Navarro M. (2012). Tephra hazard assessment at Concepciòn Volcano, Nicaragua, J. Volcanol. Geotherm. Res., Volumes 219-220, 41-51 doi:10.1016/j.jvolgeores.2012.01.007.

15. Costa A., Folch A., Macedonio G., Giaccio B., Isaia R., Smith V.C. (2012) Quantifying volcanic ash dispersal and impact from Campanian Ignimbrite super-eruption, Geophys. Res. Lett., 39, doi:10.1029/2012GL051605.

16. Bonasia R., Costa A., Folch A., Capra L., Macedonio G. (2012). Numerical simulation of tephra transport and deposition of the 1982 El Chichon eruption, J. Volcanol. Geotherm. Res., doi: 10.1016/j.jvolgeores.2012.04.006.

17. Sulpizio, R., Folch, A., Costa, A., Scaini, C., Dellino, P. (2012). Civil aviation hazard assessment of far-range volcanic ash dispersal from a violent Strombolian eruption scenario at Somma-Vesuvius volcano, Naples, Italy, Bull. Volcanol., 74, 2205-2218, doi: 10.1007/s00445-012-0656-3.

18. Collini, E., Osores, S., Folch, A., Viramonte, J.G., Villarosa, G., Salmuni, G. (2013). Volcanic ash forecast during the June 2011 Cordón-Caulle, Natural Hazards, 66(2), 389-412, doi:10.1007/s11069-012-0492-y.

19. Osores, M.S., Folch, A., Collini, E., Villarosa, G., Durant, A., Pujol, G., Viramonte, J.G. (2013). Validation of the FALL3D model for the 2008 Chaitén eruption using field, laboratory and satellite data, Andean Geology, 40 (2): 262-276.

20. Folch, A., Mingari L., Osores, M.S., Collini, E. (2013). Modeling volcanic ash resuspension. Application to the 14-18 October 2011 outbreak episode in Central Patagonia, Argentina, Nat. Hazards Earth Syst. Sci., 14, 119-133, doi:10.5194/nhess-14-119-2014.

21. Costa A., Folch A., Macedonio G. (2013) Density-driven transport in the umbrella region of volcanic clouds: Implications for tephra dispersion models, Geophys. Res. Lett., Vol. 40, 1-5, doi: 10.1002/grl.50942

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Costa, A., Folch, A., and Macedonio, G.: A model for wet aggregation of ash particles in volcanic plumes and clouds: I. Theoretical formulation, J. Geophys. Res., 115, doi:10.1029/2009JB007175, 2010.

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